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Arbitrary Order Hierarchical Bases for Computational Electromagnetics

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1 Introduction

We present a clear and general method for constructing hierarchical vector bases of arbitrary polynomial degree for use in the finite element solution of Maxwell's equations. Hierarchical bases enable p-refinement methods, where elements in a mesh can have different degrees of approximation, to be easily implemented. This can prove to be quite useful as sections of a computational domain can be selectively refined in order to achieve a greater error tolerance without the cost of refining the entire domain. While there are hierarchical formulations of vector finite elements in publication (e.g. [1]), they are defined for tetrahedral elements only, and are not generalized for arbitrary polynomial degree. Recently, Hiptmair, motivated by the theory of exterior algebra and differential forms presented a unified mathematical framework for the construction of conforming finite element spaces [2]. In [2], both 1-form (also called $H(curl)$) and 2-form (also called $H(div)$) conforming finite element spaces and the definition of their degrees of freedom are presented. These degrees of freedom are weighted integrals where the weighting function determines the character of the bases, *i.e.* interpolatory, hierarchical, etc.

In this paper we follow the work of Ciarlet [3] and define a finite element as a set of three distinct objects $(\Omega, \mathcal{P}, \mathcal{A})$ such that:

- Ω is the polyhedral domain over which the element is defined
- $\mathcal{P}$ is a finite dimensional polynomial space from which basis functions are constructed
- $\mathcal{A}$ is a set of linear functionals (*Degrees of Freedom*) dual to $\mathcal{P}$

Finite element basis functions are *not* uniquely specified until all three components of $(\Omega, \mathcal{P}, \mathcal{A})$ are defined. The finite element basis functions are a particular basis of $\mathcal{P}$ implicitly defined by the relation

$$\mathcal{A}_i(\mathbf{w}_j) = \delta_{i,j} \tag{1}$$

The key to defining hierarchical vector bases lies in the appropriate definition of the set $\mathcal{A}$ of degrees of freedom. We present a specific procedure for computing a hierarchical basis of arbitrary polynomial degree. While the approach is valid for a variety of element topologies and discrete forms, we present the procedure for 1-form bases on hexahedrons.

2 Ω - Element Topology and Geometry

We perform all computations on a reference element $\hat{\Omega}$ (all objects explicity defined on the reference element will be accented with a *hat* symbol). There exists a mapping Φ from the reference element $\hat{\Omega}$ to the actual element Ω. This mapping (defined by interpolatory *shape functions*) and its Jacobian are defined as

$$\mathbf{x} = \Phi(\hat{\mathbf{x}}); \quad \mathbf{J}_{i,j} = \frac{\partial x_j}{\partial \hat{x}_i}, \tag{2}$$

where $\hat{\mathbf{x}} \in \hat{\Omega}$ and $\mathbf{x} \in \Omega$. Unlike the approach presented in [4] and [1], we define the basis functions $\hat{\mathbf{w}}$ on the reference element and transform them as necessary during the finite element assembly procedure. We do this because the hierarchical basis functions are expensive to compute; using the following transformations the bases need only be computed once. The appropriate transformations for 1-forms and their derivative are

$$\mathbf{w} = \mathbf{J}^{-1}(\hat{\mathbf{w}} \circ \Phi); \quad d\mathbf{w} = \frac{1}{|\mathbf{J}|}\mathbf{J}^T(d\hat{\mathbf{w}} \circ \Phi) \tag{3}$$

3 $\mathcal{P}$ - Polynomial Spaces

For $\mathcal{P}$ we use the polynomial space originally proposed in [5]. Let $Q_{p_1,p_2,\ldots,p_n}$ denote a polynomial of n variables $(x_1, x_2, \ldots, x_n)$ whose maximum degree is p_1 in x_1, p_2 in x_2, ..., p_n in x_n. Using this notation, the appropriate polynomial space for a 1-form basis on the unit hexahedron is

$$\mathcal{P}^p(\hat{\Omega}) = \{\mathbf{u}; u_x \in Q_{p-1,p,p}, u_y \in Q_{p,p-1,p}, u_z \in Q_{p,p,p-1}\}; \;\; dim(\mathcal{P}^p(\hat{\Omega})) = 3p(p+1)^2 \tag{4}$$

Note that $\mathcal{P}^p(\hat{\Omega})$ does not yet define our finite element basis functions. Rather, we consider $\mathcal{P}^p(\hat{\Omega})$ to be a *primitive* space that is easily and efficiently implemented. The final hierarchical finite element basis functions are a particular basis of $\mathcal{P}^p(\hat{\Omega})$ defined by eq (1). In our implementation, this primitive space is constructed by taking tensor direct products of 1-dimensional Lagrange interpolatory polynomial sets defined on the reference interval $[0, 1]$.

4 $\mathcal{A}$ - Degrees of Freedom

The set $\mathcal{A}$ of degrees of freedom consists of linear functionals that map an arbitrary function, $\mathbf{g}$, onto the set of real numbers. The set $\mathcal{A}$ satisfies three important properties; namely

- *Unisolvence*: $\mathcal{A}$ is dual to the finite element space, *i.e.* eq (1) must hold.
- *Invariance*: Degrees of freedom remain unisolvent upon a change of variables.
- *Locality*: The trace of a basis function on a sub-simplex is determined by degrees of freedom associated *only* with that sub-simplex.

The linear functionals from $\mathcal{A}$ are defined in terms of *weighted moment integrals* over sub-simplices of the element Ω (e.g. line integrals over edges, surface integrals over faces, etc ...)[2]. If we denote a sub-simplex of an element Ω of dimension n as Ω_n, then the generalized form of the linear functional for 1-forms is given by

$$\{\mathcal{A}_i(\mathbf{g})\} = \int_{\hat{\Omega}_n} (\mathbf{g} \circ \Phi) \wedge \mathbf{J}^T \hat{q}_n, \tag{5}$$

where $\hat{q}_n$ is an $(n-1)$-form *weighting polynomial* of n-variables defined over the reference sub-simplex $\hat{\Omega}_n$. For a 1-form, we require integrals over edges, faces and the volume of the element itself. We can therefore break the set $\mathcal{A}$ into three mutually disjoint subsets

$$\{\mathcal{A}(\mathbf{g})\} = \{\mathcal{A}^e(\mathbf{g})\} \cup \{\mathcal{A}^f(\mathbf{g})\} \cup \{\mathcal{A}^v(\mathbf{g})\}, \tag{6}$$

where the letters e, f, v denote sets of integrals over edges, faces and the volume of the element Ω respectively.

In the computation of hierarchical basis functions, the degrees of freedom $\mathcal{A}$ are weighted moment integrals evaluated on the reference element. Specifically,the 1-form hexahedral edge moments have the form

$$\{\hat{\mathcal{A}}^e(\hat{\mathbf{g}})\} = \int_{\hat{e}} \hat{\mathbf{g}} \cdot (\hat{\mathbf{t}}\hat{q}); \;\; dim(\hat{\mathcal{A}}^{\hat{e}}) = 12 * p \tag{7}$$

The symbol $\hat{\mathbf{t}}$ denotes the unit tangent vector for each of the 12 edges on the reference hexahedron. In this case the weighting polynomial $\hat{q}$ is a 1-dimensional 0-form such that $\hat{q} \in Q_{p-1}$. The face moments will have the form

$$\{\hat{\mathcal{A}}^f(\hat{\mathbf{g}})\} = \iint_{\hat{f}} \hat{\mathbf{g}} \cdot (\hat{\mathbf{n}} \times \hat{\mathbf{q}}); \;\; dim(\hat{\mathcal{A}}^f) = 6 * 2p(p-1) \tag{8}$$

The symbol $\hat{\mathbf{n}}$ denotes the unit normal vector for each of the 6 faces on the reference hexahedron. In this case the weighting polynomial $\hat{\mathbf{q}}$ is a 2-dimensional 1-form (i.e. it is defined in a plane) such that $\hat{\mathbf{q}} = (\hat{q}_1, \hat{q}_2)$. In practice, these 2-dimensional 1-forms are implemented as three dimensional vectors with one component set to zero (thus designating the plane in which it is defined). The non-zero components are such that $\hat{q}_1 \in Q_{p-2,p-1}$ and $\hat{q}_2 \in Q_{p-1,p-2}$. Finally, the volume moments will have the form

$$\{\hat{\mathcal{A}}^v(\hat{\mathbf{g}})\} = \iiint_{\hat{v}} \hat{\mathbf{g}} \cdot \hat{\mathbf{q}}; \quad dim(\hat{\mathcal{A}}^v) = 3p(p-1)^2 \tag{9}$$

The weighting polynomial $\hat{\mathbf{q}}$ is a 3-dimensional 2-form such that $\hat{\mathbf{q}} = (\hat{q}_1, \hat{q}_2, \hat{q}_3)$, where $\hat{q}_1 \in Q_{p-1,p-2,p-2}$, $\hat{q}_2 \in Q_{p-2,p-1,p-2}$ and $\hat{q}_3 \in Q_{p-2,p-2,p-1}$.

For our hierarchical basis, we use weighting functions in eqs (7)-(9) that are *orthogonal*, specifically they are a variation of Legendre polynomials that are scaled and normalized over the reference interval $[0, 1]$. Figure 1 gives some visual examples of the orthogonal weighting polynomials we use. In addition, we evaluate the integrals numerically using Gaussian quadrature that is exact to order $2p$.

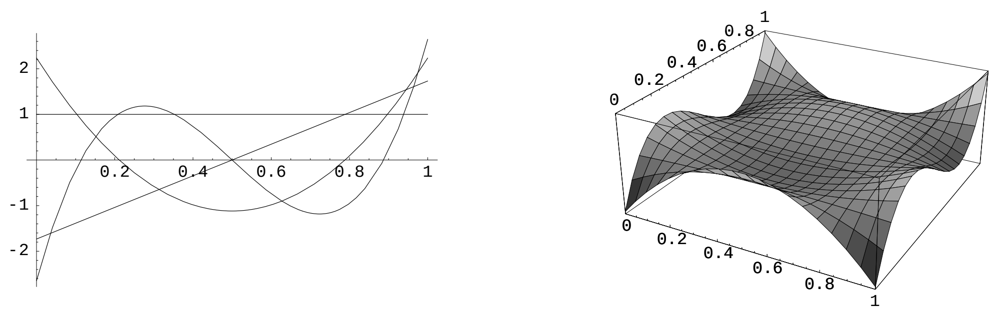

Figure 1: Examples of 1D (*left*) and 2D (*right*) orthogonal weighting polynomials

Using this general approach, we can construct a hierarchical 1-form basis of polynomial degree p in the following manner. We begin by generating a primitive basis $\{\hat{\mathbf{g}}_j\} \in G \subseteq \mathcal{P}$. Then the hierarchical basis $\{\hat{\mathbf{w}}_i\} \in W$ is expressed as a linear combination of members of the primitive basis. The key step is constructing the linear system

$$V_{i,j} = \hat{\mathcal{A}}_i(\hat{\mathbf{g}}_j); \tag{10}$$

which is similar to a Vandermonde matrix. Then, the hierarchical basis is given by

$$W = V^{-1}G \tag{11}$$

Note that V is a numerical matrix that we invert using LU decomposition. While it may seem computationally expensive to invert a matrix in order to get the hierarchical basis, it should be noted that it is a one time cost to compute the basis on the reference element. As mentioned in Section 2, the reference basis is easily mapped to actual elements via the transformation rules of eq (3).

5 Numerical Example

In this simple example we solve the vector Helmholtz equation using a hierarchical 1-form basis. The PDE in question and its discrete form are given by

$$\begin{aligned} \nabla \times \frac{1}{\mu} \nabla \times \mathbf{E} - \epsilon\omega^2 \mathbf{E} &= \mathbf{f} \qquad (12) \\ \left(A - \omega^2 B\right) x &= b \qquad (13) \end{aligned}$$

where A is the global stiffness matrix, B is the global mass matrix, b is the global load vector, and x is the unknown vector of finite element coefficients. We solve the above discrete equation using different approximation schemes and compare the resulting number of unknowns and the $L2$ approximation error. In order to compute errors, we choose an exact solution

$$\mathbf{E}(x,y,z) = \begin{cases} (1,0,x) & : \quad x < 4 \\ (1,0,1.5x^3 - 20.25x^2 + 90.25x - 132) & : \quad 4 \le x < 5 \\ (1,0,x-1) & : \quad x \ge 5 \end{cases} \tag{14}$$

and insert this into (12) to form the corresponding source function $\mathbf{f}$. Figure 2 shows a plot of the exact solution over the computational domain. The mesh consists of 9 hexahedral elements. For the first three approximation schemes, we use a hierarchical 1-form basis of polynomial degrees $p = 1, 2$ and 3 throughout the entire mesh. Because the exact solution is cubic, an $L2$ error of zero (to machine precision) is achieved using a 3^{rd} degree basis. However, using a selectively refined mesh we can achieve the same error tolerance but with far fewer unknowns. Because the basis functions are hierarchical, it is a simple matter to join the $p = 1$ elements to the $p = 3$ elements, the higher degree basis functions on the shared face joining the two elements are simply discarded. These results are summarized in Table 1.

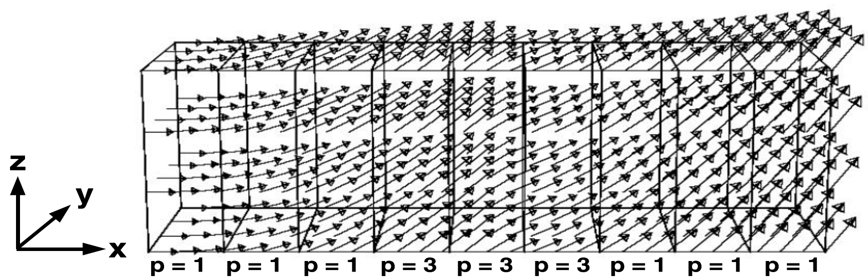

Figure 2: Function used to test hierarchical basis.

Approximation Scheme	Number of Unknowns	$L2$ Error
p = 1	60	2.55488634658e-01
p = 2	306	1.63222013549e-02
p = 3	864	1.39937249725e-14
p = 1 and 3	416	1.84362234500e-14

Table 1: Computational results for solution of vector Helmholtz equation

6 Conclusions

We have demonstrated that by properly formulating the set $\mathcal{A}$ of degrees of freedom by using orthogonal Legendre polynomials and using this set to create a linear transformation matrix, we can convert a standard interpolatory basis (or primitive basis) into a hierarchical basis. This procedure is valid for arbitrary polynomial degree and can be applied to other element topologies besides hexahedrons (i.e. tetrahedrons and prisms). The numerical benefits of a hierarchical basis were demonstrated using a simple test problem and it was shown that a significant reduction in the number of system unknowns (and hence overall computational cost) can be achieved while still maintaining the same level of accuracy by using a mesh that is selectively p-refined. Work for DOE by UC/LLNL(W-7405-Eng-48)

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